

Chemoinformatics: Theory, Practice, & Products

Barry A. Bunin, Brian Siesel, Guillermo Morales, Jürgen Bajorath



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Chemoinformatics is the use of information technology in the acquisition, analysis and management of data and information relating to chemical compounds and their properties. The purpose of this book is to provide computational scientists, medicinal chemists and biologists with complete practical information and underlying theory relating to modern Chemoinformatics and related drug discovery informatics technologies. This is an essential handbook for determining the right Chemoinformatics method or technology to use.

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